An ansatz for the eigenstates in $\mathcal{PT}$-symmetric quantum mechanics

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Abstract

We suggest a general ansatz for the energy-eigenstates when a complex one-dimensional $\mathcal{PT}$-symmetric potential possesses real discrete spectrum. Several interesting features of $\mathcal{PT}$-symmetric quantum mechanics have been brought out using this ansatz.

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The new option [1] that the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians may too have real discrete spectrum has given rise to a lot of very interesting investigations. Interestingly, in these developments exactly solvable models [2-8] have not only shown the ways but also preceded the general proofs so much that several general results are still unproved or unavailable.

The non-orthogonality of the new energy-eigenstate in the usual Hermitian sense was first encountered in exactly solvable models (e.g., [4]). Then in several independent [4,10-13] studies a new scalar product ($\mathcal{PT}$-norm, $\mathcal{PT}$-orthogonality) was proposed. Even the indefiniteness of the new norm which is well known now was first displayed only in an exactly solvable model (e.g., [9])

So far it is not stated as to when expectation values of various operators $x, f(x), p, p^2, H$ etc. under the new scalar product will be real. In the present work we provide answer to this question by assuming an ansatz for the eigenstates for a complex one-dimensional $\mathcal{PT}$-symmetric potential when it possesses real discrete spectrum.

A general $\mathcal{PT}$-symmetric Hamiltonian can be written as

$$H = \frac{p_x^2}{2m} + V_c(x) = -\frac{d^2}{dx^2} + V_0(x) + i\lambda V_1(x), \quad \hbar = 1 = 2m, \lambda\ real, \tag{1}$$

where real functions $V_0(x)$ and $V_1(x)$ are even and odd respectively. We now propose a general ansatz for the n^{th} eigenstate of the Hamiltonian (1), as

$$\Psi_n(x) = \psi_{n,0}(x) + i\psi_{n,1}(x), \quad s.t.\ \psi_{n,l}(-x) = (-)^{n+l}\psi_{n,l}(x), \tag{2}$$

where $\psi_{n,l}(x)$ are real and essentially vanish at $x = \pm\infty\ or\ \pm L$. In the above equation by noticing the novel parity scheme of $\psi_{0,1}(x)$, one can check that the eigenfunctions of all the exactly solvable models complex one-dimensional $\mathcal{PT}$-symmetric potentials conform to this interesting ansatz. In the following the indices (subscripts : $0, 1, n$) will be playing a very interesting role while appearing in the integrands of all the integrals in the sequel. If sum of these indices is even the integral will survive and will vanish otherwise.

In one dimension, when the Hamiltonian and eigenfunctions are real we can write $\mathcal{H}^* = \mathcal{H}$, $\phi_n^* = \phi_n$ and $(\mathcal{H}\phi_n)^* = \mathcal{H}^*\phi_n^* = \mathcal{H}\phi_n$ as the complex-conjugation operator does not *transpose*. In the same way, let us notice that $H^{PT} = H$ and $\Psi_n^{PT} = (-)^n\Psi_n$. Let us write the eigenvalue equation for Eqs.(1) and (2), assuming that the eigenvalues are complex $E_n = E_n^r + iE_n^i$,

$$H\Psi_n = (E_n^r + iE_n^i)\Psi_n. \tag{3}$$

Noting that if c is a constant then $(c)^{PT} = c^*$, we do $\mathcal{PT}$-operation in Eq. (3) to get

$$H\Psi_n = (E_n^r - iE_n^i)\Psi_n. \tag{4}$$

Subtracting Eq. (4) from (3), we find that $E_n^i = 0$, showing that all the eigenvalues of H are real when the $\mathcal{PT}$-symmetry is exact: the energy-eigenstate (2) is also the simultaneous eigenstate of the antiliear operator $\mathcal{PT}$.

The expectation value of an operator $\hat{O}$ is usually defined as

$$< n|\hat{O}|n >= \frac{1}{N_n}\int_{-\infty}^{\infty} \Psi_n^*(x)\ \hat{O}\ \Psi_n(x)\ dx. \tag{5}$$

When the boundary is at a finite distance, we will replace the limits by $\pm L$. Let us also define the new expectation value as

$$(n|\hat{O}|n) = \frac{1}{N'_n} \int_{-\infty}^{\infty} \Psi_n(x)\ \hat{O}\ \Psi_n(x)\ dx, \tag{6}$$

where the complex conjugation has been discreetly given up. In the following we shall be calculating both $< n|\hat{O}|n >$ and $(n|\hat{O}|n)$ for various quantal operators to compare and contrast. Since the $\mathcal{PT}$-symmetric potentials and their eigenstates corresponding to real part of the spectrum recieve increasing attention in the most recent years, the predictions as to whether the expectation value or the just defined averages of various operators would be real or imaginary, zero or non-zero and positive or negative would be valuable. In the following we will see that the proposed ansatz and the arguments based on parity of various entities would suffice to predict important results.

Let us calculate the norm, $N_n =< n|1|n >$

$$N_n = \int_{-\infty}^{\infty} \Psi^*_m(x)\Psi_n(x)\ dx = \int_{-\infty}^{\infty} [\psi^2_{n,0}(x) + \psi^2_{n,1}(x)]\ dx. \tag{7}$$

Let us also calculate a quantity $N'_n = (n|1|n)$.

$$\begin{aligned} N'_n = \int_{-\infty}^{\infty} \Psi_n(x)\Psi_n(x)\ dx &= \int_{-\infty}^{\infty} [\psi^2_{n,0}(x) - \psi^2_{n,1}(x) + 2i\psi_{n,0}(x)\ \psi_{n,1}(x)]\ dx \\ &= \int_{-\infty}^{\infty} [\psi^2_{n,0}(x) - \psi^2_{n,1}(x)]\ dx. \end{aligned} \tag{8}$$

In view of the interesting odd parity of the integrand (see Eq. (2)) the the second integral vanishes. This simply proves that $\mathcal{PT}$-norm (N'_n) will be real but indefinite (positive/negative) unlike the Hermitian norm (N_n) given in (7) which is positive definite.

Now we calculate $< n|x^{2k}|n >, k = 1, 2...$ by noticing the parity of various integrands in view of Eq.(2), we get

$$< n|x^{2k}|n >= \frac{1}{N_n} \int_{-\infty}^{\infty} x^{2k}[\psi^2_{n,0}(x) + \psi^2_{n,1}(x)]\ dx \tag{9}$$

which is real. Similarly, one can show that

$$< n|x^{2k+1}|n >= 0 \tag{10}$$

On the other hand, using a similar analysis we find that

$$(n|x^{2k}|n) = \frac{1}{N'_n} \int_{-\infty}^{\infty} x^{2k}[\psi^2_{n,0}(x) - \psi^2_{n,1}(x)]\ dx \tag{11}$$

is real. Further,

$$(n|x^{2k+1}|n) = \frac{2i}{N'_n} \int_{-\infty}^{\infty} x^{2k+1} \psi_{n,0}(x) \psi_{n,1}(x) \; dx, \tag{12}$$

which is imaginary. By noting that differentiation changes the parity of a definite parity function and that $\psi_{n,l}(\pm\infty) = 0$, we find that

$$< n|p_x|n >= \frac{2}{N'_n} \int_{-\infty}^{\infty} \psi'_{n,0}(x) \psi_{n,1}(x) \; dx, \tag{13}$$

is real while $\psi'_{n,0}(x) = \frac{d\psi_{n,0}(x)}{dx}$. But on the other hand, we find that

$$(n|p_x|n) = 0 \tag{14}$$

As the double differentiation does not change the parity of a definite parity function we use Eq.(3) to find that

$$< n|p_x^2|n >= \frac{1}{N_n} \int_{-\infty}^{\infty} [E_n - V_0(x)][\psi_{n,0}^2(x) + \psi_{n,1}^2(x)] \; dx \tag{15}$$

is real. Whereas

$$(n|p_x^2|n) = \frac{1}{N'_n} \int_{-\infty}^{\infty} \{[E_n - V_0(x)][\psi_{n,0}^2(x) - \psi_{n,1}^2(x)] + 2\lambda V_1(x) \psi_{n,0}(x) \psi_{n,1}(x)\} \; dx \tag{16}$$

is also real. Next, we find the expectation value of $V_c(x) = V_0(x) + i\lambda V_1(x)$, we have

$$< n|V_c(x)|n >= \frac{1}{N_n} \int_{-\infty}^{\infty} V_0(x)[\psi_{n,0}^2(x) + \psi_{n,1}^2(x)] \; dx \tag{17}$$

and

$$(n|V_c(x)|n) = \frac{1}{N'_n} \int_{-\infty}^{\infty} \{V_0(x)[\psi_{n,0}^2(x) - \psi_{n,1}^2(x)] - 2\lambda V_1(x) \psi_{n,0}(x) \psi_{n,1}(x)\} \; dx. \tag{18}$$

By adding Eq.(15) with Eq.(17) and Eq.(16) with Eq.(18), we prove that

$$< n|H|n >= E_n = (n|H|n). \tag{19}$$

This is a remarkable result which establishes the equality of expectation values of the Hamiltonian under the old (5) and new (6) definitions. We now take up the issue of the orthogonality of $\Psi_n(x)$. For two states $m \neq n$ with distinct eigenvalues E_m and E_n (complex or real), let us write the Schrödinger equation as

$$H\Psi_m(x) = E_m \Psi_m(x), \tag{20}$$

$$H\Psi_n(x) = E_n\Psi_n(x). \tag{21}$$

Let us left-multiply (20) by $\Psi_n(x)$ and (21) by $\Psi_m(x)$ and subtract both the equations and integrate $w.r.t.x$ to have

$$\begin{aligned} &(E_m - E_n)\int_{-\infty}^{\infty} \Psi_m(x)\Psi_n(x)\ dx \\ &= \int_{-\infty}^{\infty} [\Psi_n(x)H\Psi_m(x) - \Psi_m(x)H\Psi_n(x)]\ dx \\ &= -\int_{-\infty}^{\infty} \left\{\Psi_n(x)\frac{d^2}{dx^2}\Psi_m(x) - \Psi_m(x)\frac{d^2}{dx^2}\Psi_n(x)\right\}\ dx \\ &= \left[\Psi_n(x)\frac{d\Psi_m(x)}{dx} - \Psi_m(x)\frac{d\Psi_n(x)}{dx}\right]_{-\infty}^{\infty} \ = \ 0. \end{aligned} \tag{22}$$

The last term vanishes due to the boundary condition i.e., $\Psi_j(\pm\infty) = 0$. And so we have proved the orthogonality of two eigenstates corresponding to two distinct eigenvalues for a $\mathcal{PT}$-symmetric Hamiltonian in general. Thus, the orthogonality condition for the eigenstates (2) of an arbitrary $\mathcal{PT}$-invariant potential can now be stated as

$$(E_m - E_n)\int_{-\infty}^{\infty} \Psi_m(x)\ \Psi_n(x)\ dx = 0,\ m \neq n, \tag{23}$$

notice the absence of complex conjugation. Using Eqs. (20) and (21) and bearing in mind that the complex-conjugation does not *transpose*, we can derive

$$\begin{aligned} &(E_n - E_m)\int_{-\infty}^{\infty} \Psi_m^*(x)\Psi_n(x)\ dx = 2i\int_{-\infty}^{\infty} \Psi_m^*(x)\lambda V_1(x)\Psi_n(x)\ dx \\ &= 2\int_{-\infty}^{\infty} \lambda V_1(x)[\psi_{m,1}(x)\psi_{n,0}(x) - \psi_{m,0}(x)\psi_{n,1}(x)]\ dx, if\ m+n = even, \\ &= 2i\int_{-\infty}^{\infty} \lambda V_1(x)[\psi_{m,0}(x)\psi_{n,0}(x) + \psi_{m,1}(x)\psi_{n,1}(x)]\ dx, if\ m+n = odd. \end{aligned} \tag{24}$$

It is helpful to note that whenever $\psi_{p,q}(x)$ appears in an integral and if sum of all the indices of the integrand is even the integral survives and the integral vanishes otherwise. The Eq.(24) demonstrates that $\Psi_m(x)$ and $\Psi_n(x)$ are not orthogonal in the conventional way. For a better insight, let us see the orthogonality in another way by expressing $< m|n >$ and (m, n) as

$$\begin{aligned} < m|n > = \int_{-\infty}^{\infty} \Psi_m^*(x)\ \Psi_n(x)\ dx, = \int_{-\infty}^{\infty} \{&[\psi_{m,0}(x)\psi_{n,0}(x) + \psi_{m,1}(x)\psi_{n,1}(x)] \\ &+i[\psi_{m,0}(x)\psi_{n,1}(x) - \psi_{m,1}(x)\psi_{n,0}(x)]\}\ dx, \end{aligned} \tag{25}$$

$$(m|n) = \int_{-\infty}^{\infty} \Psi_m(x)\ \Psi_n(x)\ dx, = \int_{-\infty}^{\infty} \{[\psi_{m,0}(x)\psi_{n,0}(x) - \psi_{m,1}(x)\psi_{n,1}(x)] + i[\psi_{m,0}(x)\psi_{n,1}(x) + \psi_{m,1}(x)\psi_{n,0}(x)]\}\ dx. \tag{26}$$

A comparison of Eq. (26) with Eq. (23) leads to two interesting additional properties of $\psi_{p,q}(x)$, viz.,

$$\int_{-\infty}^{\infty} \psi_{m,0}(x)\psi_{n,0}(x)\ dx = \int_{-\infty}^{\infty} \psi_{m,1}(x)\psi_{n,1}(x)\ dx,\ m \neq n, \tag{27}$$

and

$$\int_{-\infty}^{\infty} \psi_{m,0}(x)\psi_{n,1}(x)\ dx = -\int_{-\infty}^{\infty} \psi_{m,1}(x)\psi_{n,0}(x)\ dx,\ m \neq n. \tag{28}$$

if the ansatz (2) were to represent the eigenstate of a $\mathcal{PT}$-symmetric Hamiltonian with real discrete spectrum. More importantly, notice once again that the usual orthogonality condition using the complex-conjugation would not hold as Eq. (26) does not vanish in view of properties Eqs.(27) and (28). It is crucial to note that the right hand sides of Eqs. (24) and (25) would vanish due to different set of conditions. A common but trivial condition would of course be when $\lambda = 0$ implying that the potential is real. It is also imprtant to notice that

$$\int_{-\infty}^{\infty} \psi_{n,0}^2(x)\ dx \neq \int_{-\infty}^{\infty} \psi_{n,1}^2(x)\ dx. \tag{29}$$

from Eq. (27). This means that $\mathcal{PT}$-norm (8) in case of real discrete spectrum does not vanish.

So far we have worked with the proposed ansatz (2) which represnts only the scenario when the $\mathcal{PT}$-symmetry is exact: the energy-eigenstates are also the eigenstaes of the anti-linear operator $\mathcal{PT}$ and the discrete energy-eigenvalues are real. We now consider the general case when the $\mathcal{PT}$-symmetry could be broken or unbroken. By operating with $\mathcal{PT}$ in both the sides and remembering that $(c)^{PT} = c^*$ and the fact that complex-conjugation does not *transpose*, using Eqs. (20,21) we find that

$$(E_m^* - E_n) \int_{-\infty}^{\infty} \Psi_m^{PT}(x)\Psi_n(x)\ dx = \int_{-\infty}^{\infty} [\Psi_n(x) H \Psi_m^{PT}(x) - \Psi_m^{PT}(x) H \Psi_n(x)]\ dx$$

$$= -\int_{-\infty}^{\infty} \left\{ \Psi_n(x) \frac{d^2}{dx^2} \Psi_m^{PT}(x) - \Psi_m^{PT}(x) \frac{d^2}{dx^2} \Psi_n(x) \right\} dx,$$

$$= \left[\Psi_n(x) \frac{d\Psi_m^{PT}(x)}{dx} - \Psi_m^{PT}(x) \frac{d\Psi_n(x)}{dx} \right]_{-\infty}^{\infty} = 0. \qquad (30)$$

It is could be instructive to notice that the just derived orthogonality condition i.e.,

$$(E_m^* - E_n) \int_{-\infty}^{\infty} \Psi_m^{PT}(x)\ \Psi_n(x)\ dx = 0. \qquad (31)$$

is more general as it degenerates to (24) when the $\mathcal{PT}$-symmetry is unbroken i.e., $\Psi^{PT}(x) = (-)^n \Psi(x)$, and the eigenvalues are real, ($E_m^* = E_m$). When $m = n$ and $\Psi_m(x)$ are no more eigenstates of $\mathcal{PT}$, the $\mathcal{PT}$-symmetry is broken and eigenvalues are complex conjugate pairs and consequently according to Eq. (31) the $\mathcal{PT}$-norm vanishes. Such states are also termed as self-orthogonal states [14]. Following the suggestions in Refs. [4,10-13], we could have also defined the expectation value $(n|\hat{O}|n)$ (8) alternatively as

$$(n|\hat{O}|n) = \frac{1}{N_n'} \int_{-\infty}^{\infty} \Psi_n^{PT}(x) \hat{O} \Psi_n(x)\ dx, N_n' = \int_{-\infty}^{\infty} \Psi_n^{PT}(x) \Psi_n(x)\ dx. \qquad (32)$$

Since $\Psi_n^{PT}(x) = (-)^n \Psi_n(x)$ in the case of the real discrete spectrum, the above results remain unchanged. An interesting account of the definition of the expectation (6) in the light of bi-orthogonality can be found in a very recent work [15].

The results proved in Eqs. (9-12,14,16,18) can be summarized by stating that in $\mathcal{PT}$-symmetric quantum mechanics only $\mathcal{PT}$-symmetric operators can have real expectation values. This means the expectation values of ix and e^{ix} will be real. This is akin to the conventional Hermitian quantum mechanics wherein only Hermitian operators have real eigenvalues. The result in Eq. (19) is interestingly surprising which states that expectation value of the complex $\mathcal{PT}$-symmetric Hamiltonian remains equal to the energy eigenvalue irrespective of the definitions of the expectation value given in Eq. (5) and (6). This means the variational method [10] can work for the new Hamiltonians under both old and new definitions. We remark that these results have not appeared before. Eq.(8) proves the indefiniteness of the $\mathcal{PT}$-norm. Importantly, Eq. (29) proves that in the case of unbroken $\mathcal{PT}$-symmetry (real discrete spectrm) the new norm does not vanish.

We would like to re-emphasize that all these results could be proved merely by the parity scheme of the suggested ansatz for the energy-eigenfunction in Eq. (2). It may be verified that the energy-eigenfunction of all the exactly solvable one-dimensional models of the complex $\mathcal{PT}$-symmetric potentials essentially conform to the suggested ansatz (2).

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